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Thermalization in systems with bipartite eigenmode entanglement

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Abstract. It is analytically shown that the asymptotic correlations following a quantum quench in exactly solvable models can sometimes look essentially thermal provided the initial coupling between the system eigenmodes induces a large gap. We study this phenomenon using simple models, which also illustrate the relationship between the entanglement spectrum of the initial state and the generalized Gibbs ensemble describing the long-time correlations after the quench. We also show that the effective temperature characterizing the correlations is not related to the energy fluctuations after the quench, and therefore does not have thermodynamic meaning. The latter observation implies a breakdown of the fluctuation–dissipation theorem.

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Contents

1. Introduction

Experiments with ultracold gases [1–5] and, in particular, the ongoing efforts to build quantum emulators using ultracold atoms loaded in optical lattices, have generated much interest in understanding the thermalization mechanisms of integrable models [1, 6–13]. The latter can be used as simple systems to validate a quantum emulator by comparing the outcome of the experiment to the exact solution, prior to using the emulator to study other, more complex models, for which no exact solutions are known.

However, in order to understand the outcome of a simulation of an integrable or exactly solvable model it is important to understand the effect of the initial conditions. Since quantum emulators of ultracold atoms are largely isolated systems and its evolution is essentially unitary, it becomes necessary to understand the conditions under which the asymptotic state of the system can be described by a standard statistical (i.e. Gibbsian) ensemble, or, as was pointed out recently by Rigol *et al* [6], must be described by a generalized Gibbs ensemble (GGE). The latter captures the fact that the existence of a non-trivial set of integrals of motion strongly constrain the non-equilibrium dynamics of the system.

In [12] (see also [14], for a discussion applying to local observables), we showed that the GGE can be analytically derived for exactly solvable models and a general class of initial states. In particular, we showed that dephasing between different modes makes equal time correlation functions of both local and non-local operators non-ergodic, in the sense that in the thermodynamic limit, their infinite time limit only depends on the occupation of the eigenmodes in the initial state. Thus, the asymptotic values of those correlation functions can be equivalently obtained by assuming that the correlations with other eigenmodes produce an effective temperature. This yields a description of the asymptotic correlations that is entirely equivalent to the GGE.

Nevertheless, it was also noted in [7, 8] that certain kinds of initial states can lead to asymptotic values of the observables that are essentially indistinguishable from those computed with a standard thermal Gibbs ensemble (TGE). Other cases of (pre-) thermalization have been found in integrable [15] and non-integrable [16–18] systems for particular classes of initial conditions. Recently, Mitra and Giamarchi [19] also showed that the adiabatic introduction of a nonlinearity following a quantum quench in the Luttinger model (LM), can lead to thermalization as described by the standard Gibbs ensemble. The authors of [19] emphasized the importance of 'mode coupling' for thermalization. Furthermore, a pre-thermalized regime characterized by an effective temperature was recently observed experimentally and also theoretically analyzed by the authors of [18]. Other theoretical studies [20] have also found regimes in which correlations can appear essentially thermal in various kinds of systems.

In this work, we show that for certain classes of quenches for which two sets of modes are strongly entangled in the initial state, the GGE ensemble can be arbitrarily close to the standard thermal Gibbs ensemble. Using the methods of [12], we find a simple instance of the mechanism by which initial states can lead to correlations that essentially look thermal. As we show below, this happens when the eigenmodes of the Hamiltonian that describes the evolution of a system following a quantum quench have a certain kind of bi-partite quantum correlation (i.e. entanglement) in the initial state. As an application, we find an analytical explanation for the numerical observations first reported in [7]. This fact could be used as a simple protocol to produce asymptotic correlations that essentially look like (rather high-temperature) thermal correlations in exactly solvable systems. Furthermore, we will show below that the effective temperature that characterizes the asymptotic thermal correlations can be related to the entanglement spectrum of a subset of entangled modes, which means that the latter is accessible experimentally by measuring the effective temperature that characterizes the correlations at long times after the quench.

Before illustrating the above claim, let us first describe the general set up that will be addressed below. We also want to provide a brief review of the results of [12] and discuss the relevance of quantum quenches to the theory of quantum entanglement. Re-interpreting the results of [12] in the language of entanglement theory will allow us to establish an interesting connection between the GGE introduced in [6] and the concept of entanglement spectrum [21]. This connection, along with the results of [29], will suffice to demonstrate the existence of thermal-like correlations after a quantum quench.

Consider a system containing two subsystems A and B that are initially coupled together. For times $t \leqslant 0$, the system is described by a Hamiltonian of the form $H_0 = H_A + H_B + H_{AB}$, where H_A, H_B and H_{AB} are quadratic in some eigenmodes $\{a_k, b_k\}$ which carry a quantum number k (which forms a continuum in the thermodynamic limit) and can be fermionic or bosonic, i.e.

$$H_A = \sum_k \varepsilon_A(k) a_k^\dagger a_k, \tag{1}$$

$$H_B = \sum_k \varepsilon_B(k) b_k^\dagger b_k, \tag{2}$$

$$H_{AB} = \sum_k \Delta_{AB}(k) \left[a_k^\dagger b_k + b_k^\dagger a_k \right]. \tag{3}$$

The dispersion relations are assumed such that $\epsilon_A(k) \neq \epsilon_B(k)$ for essentially all k, which is required (see below) for dephasing between the two subsystems to occur as $t \to +\infty$. We can assume that the system is prepared in an initial state in contact with a thermal reservoir at a temperature T, i.e. $\rho_0 = Z_0^{-1}\, \mathrm{e}^{-H_0/T}$ (such that $\mathrm{Tr}\, \rho_0 = 1$). For $t > 0$, the coupling between the two subsystems H_{AB} disappears, and the two subsystems evolve unitarity and are uncoupled, according to the Hamiltonian:

$$H = H_A + H_B. \tag{4}$$

The existence of the coupling H_{AB} for all $t \leqslant 0$ implies that in the initial state, ρ_0, there are correlations (i.e. bi-partite entanglement) between the eigenmodes, i.e. $\langle a_k^\dagger b_k \rangle \neq 0$.

According to the conjecture of Rigol *et al* [6], the asymptotic state of the system can be described by a GGE density matrix that is obtained using the maximum entropy principle taking into account that the system dynamics is constrained by the existence of the set of integrals of motion given by $I_a(k) = a^\dagger(k)a(k)$ and $I_b(k) = b^\dagger(k)b(k)$. The GGE density matrix thus obtained reads:

$$\rho_{\mathrm{GGE}} = Z_{\mathrm{GGE}}^{-1} \exp\left\{-\sum_k \left[\alpha(k)a_k^\dagger a_k + \beta(k)b_k^\dagger b_k\right]\right\}, \tag{5}$$

where the Lagrange multipliers are determined by the initial conditions, i.e. $\alpha(k) = \ln[(1 \pm n^a(k))/n^a(k)]$ and $\beta(k) = \ln[(1 \pm n^b(k))/n^b(k)]$, with $n^a(k)$ and $n^b(k)$ given by (9) and (10) (the + applies to bosonic and the − to fermonic modes).

Alternatively, one can arrive at an equivalent result by a different route [12]. Let us first consider the expansion of a local operator in terms of the eigenmodes of H:

$$O(x,t) = \sum_k \left[\phi_k^A(x)\, \mathrm{e}^{-\mathrm{i}\varepsilon_A(k)t} a_k + \phi_k^B(x)\, \mathrm{e}^{-\mathrm{i}\varepsilon_B(k)t} b_k\right]. \tag{6}$$

At asymptotically long times after the quantum quench, provided $\epsilon_A(k) \neq \epsilon_B(k)$ and certain conditions of smoothness are met, dephasing renders the two-point correlation function $\langle O^\dagger(x,t)O(0,t)\rangle$ to the following form [12]:

$$\lim_{t\to\infty} \langle O^\dagger(x,t)O(0,t)\rangle = \sum_k \left[\phi_k^A(x)\right]^* \phi_k^A(0)\langle a_k^\dagger a_k\rangle + \sum_k \left[\phi_k^B(x)\right]^* \phi_k^B(0)\langle b_k^\dagger b_k\rangle, \tag{7}$$

Thus, we see that the asymptotic correlations of $O(x)$ depend only on the eigenmode occupation in the initial state, behavior that has been termed non-ergodic in [12]. The above sum over k in equation (7) allows us to define a mode-dependent temperature for each mode [12]. Indeed, this statement is equivalent to the GGE (cf equation (5)) for a broad class of (Gaussian) initial states (see [12] and below). Thus, it follows that:

$$\lim_{t\to+\infty} \langle O^\dagger(x,t)O(0,t)\rangle = \langle O^\dagger(x)O(0)\rangle_{\mathrm{GGE}}. \tag{8}$$

The above result, valid for local operators, can be combined with Wick's theorem to show that the asymptotic behavior of non-local operators (i.e. operators whose correlation functions can be expressed as polynomials of the correlation functions of local operators) is also described by the GGE [12].

Alternatively, when the correlations are bi-partite, we can regard the effective temperature for the modes in the subsystem A as due to their entanglement with the modes in the subsystem B (and vice versa). Thus, whenever we are dealing with $\langle a_k^\dagger a_k\rangle = \mathrm{Tr}\,\rho_0 a_k^\dagger a_k$ or $\langle b_k^\dagger b_k\rangle = \mathrm{Tr}\,\rho_0 b_k^\dagger b_k$, we can trace out one of the subsystems, and write

$$n^a(k) = \langle a_k^\dagger a_k\rangle = \mathrm{Tr}\,\rho_A a_k^\dagger a_k = \mathrm{Tr}\,\rho_{\mathrm{GGE}}\, a_k^\dagger a_k, \tag{9}$$

$$n^b(k) = \langle b_k^\dagger b_k\rangle = \mathrm{Tr}\,\rho_B b_k^\dagger b_k = \mathrm{Tr}\,\rho_{\mathrm{GGE}}\, b_k^\dagger b_k, \tag{10}$$

where $\rho_A = \mathrm{Tr}_B\rho_0$ and $\rho_B = \mathrm{Tr}_A\rho_0$. Therefore, the GGE density matrix can be written as

$$\rho_{\mathrm{GGE}} = \rho_A \otimes \rho_B. \tag{11}$$

We can regard the result in equation (11) as a way to relate the density matrix of the GGE ensemble to the reduced density matrices of the subsystems A and B. Furthermore, since both ρ_A and ρ_B are Hermitian, it is possible to write these objects as follows [21, 22]:

$$\rho_{A(B)} = \frac{\mathrm{e}^{-\mathcal{H}_{A(B)}}}{Z_{A(B)}}, \tag{12}$$

where we have introduced the entanglement Hamiltonian of the A (B) subsystem $\mathcal{H}_{A(B)}$, which is also a Hermitian operator. Thus, we see ρ_{GGE} is determined by the total entanglement Hamiltonian, $\mathcal{H} = \mathcal{H}_A + \mathcal{H}_B$.

The reduced density matrix describing a subsystem A of either a pure state or a thermal mixed state plays an important role in quantum information theory applied to condensed matter systems [21]. For a pure state, the von Neumann entropy $S_A = -\mathrm{Tr}\,\rho_A \log_2 \rho_A$ measures the entanglement between two subsystems A and B. The latter can be expressed in terms of the entanglement spectrum of $\mathcal{H}_A$. Recently, the von Neumann entropy and entanglement spectrum have become an important tool, as they can be used to characterize topological quantum phases in various kinds of quantum systems, such as graphene [23], topological insulators [24] and quantum spin chains [25]. In this context, an important question that has been addressed in recent times is that the conditions under the entanglement Hamiltonian $\mathcal{H}_A$ can be proportional to the subsystem Hamiltonian H_A. Some examples of this fact have been discussed in the literature [24, 26–29]. As we show in the example below (see section 2), when this happens to be the case in a system like the one described above, we can expect the asymptotic correlations after the quantum quench to become essentially thermal.

Using the methods of [30], the entanglement Hamiltonian $\mathcal{H}_{A(B)}$ can be determined for a (Gaussian) initial state of the form $\rho_0 = Z_0^{-1}\mathrm{e}^{-H_0/T}$ ($\rho_0 = |\Phi_0\rangle\langle\Phi_0|/\langle\Phi_0|\Phi_0\rangle$, where $|\Phi_0\rangle$ is the ground state of H_0 at $T=0$). Thus [29],

$$\mathcal{H}_A = \sum_k \ln\left[(1 \pm n^a(k))/n^a(k)\right] a_k^\dagger a_k, \tag{13}$$

$$\mathcal{H}_B = \sum_k \ln\left[(1 \pm n^b(k))/n^b(k)\right] b_k^\dagger b_k, \tag{14}$$

which, by comparison with equation (5), allows us to identify the Lagrange multipliers $\alpha(k)$ and $\beta(k)$ of the GGE with the entanglement spectrum of the subsystems A and B.

Thus, the entanglement spectrum determines the asymptotic state following a quantum quench. Similar ideas have been discussed by Qi *et al* [24] for the particular case of two coupled edge states using boundary conformal field theory. Conversely, provided the Lagrange multipliers $\alpha(k)$ and $\beta(k)$ could be determined experimentally, we would be able to access the entanglement spectrum and the von Neumann entropy of the subsystems A and B. However, in actual experiments it may be difficult to obtain the full functional dependence of $\alpha(k)$ and $\beta(k)$. Thus, below we shall focus on two cases where the entanglement spectrum takes a simple form, which may be easier to measure experimentally.

The rest of this work is organized as follows. In the following section, using the above results, we provide an example of the case in which the asymptotic correlations are essentially thermal, which we show to be a consequence of the entanglement Hamiltonians $\mathcal{H}_{A(B)}$ to be proportional to the subsystem Hamiltonian, $H_{A(B)}$. In section 3, we provide a counter-example of the fact that bi-partite entanglement does not always lead to thermal correlations. This counter-example illustrates the observation that thermal correlations appear provided bi-partite entanglement arises from a gap in the spectrum of the Hamiltonian that determines the initial state. Finally, in section 4, we provide a discussion of our results and show that, even when the correlations look essentially thermal, there are certain observables like energy fluctuations that still differ from their thermal values, a fact that signals a breakdown of the fluctuation–dissipation theorem in the asymptotic state. The appendix contains some technical details regarding a continuum version of the model discussed in section 2.

2. Example

Let us first consider a model that has been numerically studied earlier by Rigol *et al* [7]. The model describes a system of hard-core bosons in one-dimensional (1D) that initially (i.e. for $t \leqslant 0$) move in the presence of superlattice potential. The hard-core bosons in 1D can be treated using a Jordan Wigner transformation [31, 32], which maps the hard-core bosons to non-interacting fermions and, in the case of a superlattice of strength Δ, leads to the following quadratic Hamiltonian:

$$H_0 = -\sum_{j=1}^{L}\left(f_j^\dagger f_{j+1} + f_{j+1}^\dagger f_j\right) + \Delta\sum_{j=1}^{L}(-1)^j f_j^\dagger f_j, \tag{15}$$

where $f_j^\dagger$ and f_j are creation and annihilation operators for spinless fermions at site j ($j = 1, \ldots, L$, for a lattice of L sites). Rigol *et al* [7] numerically found that, starting from the ground state of H_0, if the superlattice term $\propto \Delta$ is suddenly switched off at $t = 0$, and the system is allowed to evolve unitarity according to

$$H = -\sum_{j=1}^{L}\left(f_j^\dagger f_{j+1} + f_{j+1}^\dagger f_j\right), \tag{16}$$

the long-time behavior of the momentum distribution can be described by a standard Gibbs canonical ensemble,

$$\rho = \frac{1}{Z}\,\mathrm{e}^{-H/T_{\mathrm{eff}}}, \tag{17}$$

for which the effective temperature, T_{eff}, was found to approach $\Delta/2$ for $\Delta \gtrsim 1$. In what follows, we will analytically demonstrate that this numerical observation indeed follows from the existence of a strong bi-partite entanglement between two sets of eigenmodes of H.

We begin by Fourier transforming H_0 and H by using[8]

$$f_k = \frac{1}{\sqrt{L}}\sum_{j=1}^{L}\mathrm{e}^{-\mathrm{i}kx_i} f_i, \tag{18}$$

[8] We use periodic boundary conditions here, whereas Rigol *et al* used open boundary conditions [7]. The difference is irrelevant in the thermodynamic limit, where the methods of [12] apply.

with $x_j = j$, the Hamiltonian (15) can be written as

$$H_0 = H + \Delta \sum_k \left(f_k^\dagger f_{k+\pi} + f_{k+\pi}^\dagger f_k \right), \tag{19}$$

$$H = \sum_k \omega_k \left(f_k^\dagger f_k - f_{k+\pi}^\dagger f_{k+\pi} \right) \tag{20}$$

where $\omega_k = -2\cos k$ and $-\pi/2 < k \leqslant \pi/2$. The Hamiltonian describes the state of the system at $t < 0$, namely H_0, can be brought to diagonal form by means of the following canonical transformation:

$$\gamma_k = \cos\theta_k f_k + \sin\theta_k f_{k+\pi}, \tag{21}$$

$$\delta_k = -\sin\theta_k f_k + \cos\theta_k f_{k+\pi}, \tag{22}$$

with $\tan 2\theta_k = \frac{\Delta}{\omega_k}$. Hence,

$$H_0 = \sum_k E_k \left(\gamma_k^\dagger \gamma_k - \delta_k^\dagger \delta_k \right), \tag{23}$$

where $E_k = \sqrt{\omega_k^2 + \Delta^2}$. Note that the transformation in (21) and (22) implies the existence of strong bi-partite quantum correlations (i.e. entanglement) between the modes at k and $k+\pi$, which manifest in, e.g., $\langle f_k^\dagger f_{k+\pi} \rangle = -\frac{1}{2}\sin 2\theta_k = -\frac{\Delta}{2E_k} \neq 0$.

As discussed in [9, 12], the asymptotic momentum distribution of the hardcore bosons for $t \to +\infty$ can be obtained from the Fourier transform of the one-particle correlation function of the bosons, which in turn can be written as a Toeplitz determinant involving correlation two-point correlations of the Jordan–Wigner fermions:

$$\lim_{t\to+\infty} g^{(1)}(x_i - x_j, t) = \begin{vmatrix} a_0 & a_1 & \cdots & a_{-n+1} \\ a_1 & a_0 & \cdots & a_{-n+2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1} & a_{n-2} & \cdots & a_0 \end{vmatrix}, \tag{24}$$

where

$$a_{i-j+1} = -\lim_{t\to+\infty} \langle A_i(t) B_j(t) \rangle. \tag{25}$$

The thermodynamic limit is implicitly understood in the above expressions; we have also introduced the notations: $A_j = f_j^\dagger + f_j$ and $B_j = f_j^\dagger - f_j$. The above correlation function of the (local) operators A_i and B_j can be shown to be:

$$a_{i-j+1} = \frac{1}{L} \sum_k \mathrm{e}^{-\mathrm{i}k(x_i - x_j)} \left[2n(k) - 1\right] + \frac{(-1)^{i-j}}{L} \sum_k \mathrm{e}^{-\mathrm{i}k(x_i - x_j)} \left[2n(k+\pi) - 1\right] \tag{26}$$

Next, we use ($K = 0, \pi$):

$$n(k+K) = \langle f_{k+K}^\dagger f_{k+K} \rangle = \mathrm{Tr}\, \rho_0 f_{k+K}^\dagger f_{k+K}, \tag{27}$$

$$= \mathrm{Tr}\, \rho_K\, f_{k+K}^\dagger f_{k+K}, \tag{28}$$

where $\rho_0 = |\Phi_0\rangle\langle\Phi_0|$, $|\Phi_0\rangle$ being the initial state, that is, the ground state of H_0 (cf equation (15)) and the reduced density matrices:

$$\rho_K = \mathrm{Tr}_{k\in S_K}\, \rho_0, \tag{29}$$

where $S_0 = (-\pi/2, +\pi/2]$ and $S_\pi = (-\pi, +\pi] - S_0$. In other words, the asymptotic correlations can be obtained from the reduced density matrix resulting from tracing one of the two sets of entangled modes with k belonging to either S_0 or S_π.

As explained in section 1, the reduced matrices $\rho_{K=0,\pi}$ can be obtained analytically in terms of the occupation numbers of $n(k+K) = \langle f^\dagger_{k+K} f_{k+K}\rangle$ in the initial state. Using (21) and (22), we find:

$$n(k) = \frac{1}{2}\left(1 - \frac{\omega_k}{E_k}\right), \tag{30}$$

$$n(k+\pi) = \frac{1}{2}\left(1 + \frac{\omega_k}{E_k}\right), \tag{31}$$

and, following the discussion in section 1, the Lagrange multipliers determining the GGE density matrix read:

$$\begin{aligned} \alpha(k) &= \ln\left[(1-n(k))/n(k)\right] \\ &= \ln\left[\frac{E_k+\omega_k}{E_k-\omega_k}\right], \\ \beta(k) &= \ln\left[(1-n(k+\pi))/n(k+\pi)\right] \\ &= \ln\left[\frac{E_k-\omega_k}{E_k+\omega_k}\right]. \end{aligned} \tag{32}$$

For $\Delta \gg \omega_k$, E_k can be approximated by Δ, and therefore $\alpha(k) \simeq 2\omega_k/\Delta \simeq -\beta(k)$. Thus, the GGE density matrix, equation (5), reduces to a standard Gibbs ensemble, equation (17), with

$$T_{\text{eff}} \simeq \Delta/2, \tag{33}$$

which is in agreement with the numerical observations of Rigol *et al* [7]. However, it is important to note that the above thermal ensemble and the result of equation (33) is only an approximation to the actual GGE ensemble determined by the Lagrange multipliers in equation (32). However, this approximation becomes better and better for larger values of Δ, which implies that numerically (and experimentally) the GGE and a standard TGE will be essentially indistinguishable.

It is worth noting that the above results are also relevant for a special limit of an integrable field theory in one dimension, namely the sine-Gordon model:

$$H_{\text{sG}} = H_0 - \frac{vg}{\pi a_0^2}\int \mathrm{d}x \cos 2\phi, \tag{34}$$

$$H_0 = \frac{v}{2\pi}\int \mathrm{d}x\left[K^{-1}(\partial_x\phi)^2 + K(\partial_x\theta)^2\right], \tag{35}$$

where a_0 is a short-distance cutoff, and the phase and density fields $\theta(x)$ and $\phi(x)$, are canonically conjugated in the sense that they obey: $[\phi(x), \partial_{x'}\theta(x')] = \mathrm{i}\pi\delta(x-x')$; v is the speed of sound and K is a dimensionless parameter that determines the ground correlations of the system. Indeed, in equilibrium, the model exhibits two phases for $g > 0$, namely, a gapped phase for $K < 2$ and gapless phase for $K \geqslant 2$ [31]. For $K = 1$, as described in the appendix, this model can be mapped onto a model of massive fermions in 1D:

$$H_{\rm sG} = \sum_p \varepsilon_p^0 \left[\psi_{\rm R}^\dagger(p)\psi_{\rm R}(p) - \psi_{\rm L}^\dagger(p)\psi_{\rm L}(p)\right] + \Delta \sum_p \left[\psi_{\rm R}^\dagger(p)\psi_{\rm L}(p) + \psi_{\rm L}^\dagger(p)\psi_{\rm R}(p)\right], \tag{36}$$

with $\varepsilon_p^0 = vp$ and $\Delta \propto g$. The model in equation (36) can be regarded as the continuum limit of the model of equation (19).

For larger values of the gap, $\Delta \gg va_0^{-1}$, the multipliers $\alpha(p)$ and $\beta(p)$ (see calculation in the appendix) become proportional to the dispersion relation of the Hamiltonian that governs the time evolution, $\pm\varepsilon_p^0$, respectively, with an effective temperature $T_{\rm eff}$ (it is the same for the two branches of fermions) given by

$$T_{\rm eff} = \frac{\Delta}{2\tanh\frac{\Delta}{2T}}. \tag{37}$$

We note that the effective temperature depends on the temperature of the initial thermal state. This effective 'final' temperature is always higher than the initial temperature because it contains the bi-partite entanglement between k modes. For high initial temperatures the effective temperature to which the system thermalizes is the same as the initial one. In the case of a zero-temperature initial state, the effective temperature results in $T_{\rm eff} = \Delta/2$ similar to the case of the XY model studied previously.

Generally speaking, the analysis described above is also related to the discussion of the conditions under which the entanglement Hamiltonian $\mathcal{H}_{A(B)}$ and the Hamiltonian of the subsystem $H_{A(B)}$ are (approximately) proportional to each other. If this is the case, then, according to the discussion of section 1, the GGE density matrix, equation (5), will be well approximated by the thermal density matrix of (17). Indeed, recently, Peschel and Chung [29] addressed the problem of the proportionality between $\mathcal{H}_{A(B)}$ and $H_{A(B)}$. By considering a model of two species of fermions with opposite dispersion ω_k and coupling Δ, which leads to an energy spectrum for the coupled system with a gap of magnitude 2Δ. Using the perturbation theory, they showed for $\Delta \gg \omega_k$ that $\mathcal{H}_A \simeq 2/\Delta \sum_k \omega_k a_k^\dagger a_k = (2/\Delta) H_A$ and $\mathcal{H}_B \simeq 2/\Delta \sum_k (-\omega_k) b_k^\dagger b_k = (2/\Delta) H_B$. These relations can be obtained under two conditions for the initial Hamiltonian: (i) there is only coupling to excited states with the same gap 2Δ; (ii) H_A and H_B are identical. These two conditions are the constraints for obtaining an effective temperature. The thermal correlations obtained here can be thus regarded as a direct consequence of this result when we apply it to a quantum quench where the coupling Δ is switched off at $t = 0$ and we exploit the relationship between the GGE and the reduced density matrices $\rho_{A(B)}$ described in section 1.

Another interesting consequence of the above result is the possibility to use quantum quenches to prepare systems with exactly solvable dynamics in states whose correlations will become indistinguishable from thermal correlations after the quench. However, it is unfortunate that the requirement of a large gap (i.e. the condition that $\Delta \gg 1$), implies that thermal states that can be thus obtained are characterized by extremely high effective temperatures (cf equation (33)).

3. Counter-example

The above result on the emergence of thermal behavior at long times can be regarded as a consequence of the existence of a strong bi-partite entanglement (i.e. quantum correlations) in the initial state. However, as we show in this section, the existence of such entanglement is not a sufficient condition for the emergence of thermal correlations. Indeed, if the initial state is gapless, no thermal behavior can be expected even for large coupling that generates strong entanglement. The LM [30] is one such example, as we show below.

Let us consider a quantum quench in the LM [10]. The initial state is assumed to be a mixed thermal state $\rho_0 = Z_0^{-1} \mathrm{e}^{-H_0^{\mathrm{LM}}/T}$. The initial Hamiltonian $H_0^{\mathrm{LM}} = H + H_{\mathrm{int}}$, where

$$H^{\mathrm{LM}} = \frac{2\pi v_{\mathrm{F}}}{L} \sum_{k>0} \rho_{\mathrm{R}}(k)\rho_{\mathrm{R}}(-k) + \rho_{\mathrm{L}}(-k)\rho_{\mathrm{L}}(k), \tag{38}$$

$$H_{\mathrm{int}} = \frac{\Delta}{L} \sum_{k>0} \rho_{\mathrm{R}}(k)\rho_{\mathrm{L}}(-k) + \rho_{\mathrm{R}}(-k)\rho_{\mathrm{L}}(k). \tag{39}$$

In the above expression, $\rho_{\mathrm{R(L)}}$ is the density of the right (left) moving fermions in the LM, which propagate with Fermi velocity (v_{F}) [10]. The densities obey the commutation rule $[\rho_\alpha(k), \rho_\beta(k')] = kL/2\pi\, \delta_{k+k'}\delta_{\alpha,\beta}$ ($\alpha, \beta = R, L$). Therefore, we can define two pairs of bosonic operators: $\rho_{\mathrm{L}}(k) = \sqrt{kL/2\pi}\, a_k^\dagger$, $\rho_{\mathrm{R}}(k) = \sqrt{kL/2\pi}\, b_k^\dagger$ and $\rho_{\mathrm{L}}(-k) = \rho_{\mathrm{L}}^\dagger(k)$, $\rho_{\mathrm{R}}(-k) = \rho_{\mathrm{R}}^\dagger(k)$. Thus, the Hamiltonian describing the system at $t < 0$ can be written as

$$H_0^{\mathrm{LM}} = \sum_{k>0} \left[v_{\mathrm{F}} k (a_k^\dagger a_k + b_k^\dagger b_k) + \frac{\Delta}{2\pi} k (a_k^\dagger b_k^\dagger + a_k b_k) \right]. \tag{40}$$

Note that the LM is different from the example that has been discussed in section 2 because the term that couples the two subsystems is proportional to k, while in the previous example (cf equation (15)) it was a constant. This makes the Hamiltonian H_0^{LM} gapless, as we show in the following paragraph. In the language of the renormalization group (RG), which applies to equilibrium phenomena, the above perturbation (the second term in equation (40)) is marginal and it does not open a spectral gap. This is to be contrasted with the situation studied in the previous example, where the term that is being switched is a relevant (in the RG sense) perturbation. We shall come back to the relevance of this classification further below.

A standard way to diagonalize (40) is to introduce a bosonic canonical transformation: $A_k = \cosh\phi_k a_k - \sinh\phi_k b_k^\dagger$ and $B_k = -\sinh\phi_k a_k + \cosh\phi_k b_k^\dagger$. Choose $\tanh(2\phi_k) = -\Delta/2\pi$. The initial Hamiltonian now reads

$$H_0^{\mathrm{LM}} = \sum_{k>0} \Omega_k (A_k^\dagger A_k + B_k^\dagger B_k), \tag{41}$$

where $\Omega_k = v_{\mathrm{F}} k \sqrt{(1 - (\Delta/2\pi v_{\mathrm{F}})^2)}$. Thus, the energy spectrum of H_0^{LM} is gapless.

According to the discussion of section 1 and using the methods of [12], after turning off the interaction described by $H_{\mathrm{int}} \propto \Delta$ at $t = 0$, the asymptotic behavior of the correlations can be described by a GGE matrix, which can be written as ρ_{GGE} as in equation (5) with $\alpha(k)$ and $\beta(k)$ given by the entanglement spectrum of the subsystems A and B, of modes $a_k, a_k^\dagger$ and $b_k, b_k^\dagger$, respectively.

The occupation numbers are: $n^a(k) = n^b(k) = \sinh^2(\phi_k) = 1/2(v_{\mathrm{F}} k/\Omega_k - 1)$. Hence, $\alpha(k)$ and $\beta(k)$ in equation (5) are:

$$\alpha(k) = \ln\left(\frac{v_{\mathrm{F}} k + \Omega_k}{v_{\mathrm{F}} k - \Omega_k}\right) = \varepsilon, \tag{42}$$

$$\beta(k) = \ln\left(\frac{v_{\mathrm{F}} k + \Omega_k}{v_{\mathrm{F}} k - \Omega_k}\right) = \varepsilon, \tag{43}$$

where $\varepsilon = 2[\ln(2\pi v_{\rm F}/\Delta + \sqrt{(2\pi v_{\rm F}/\Delta)^2 - 1})]$ is a constant. Hence, the entanglement Hamiltonians take the form: $\mathcal{H}_A = \sum_k \varepsilon a^\dagger a_k$ and $\mathcal{H}_B = \sum_k \varepsilon b^\dagger b_k$. Thus, we find that $\mathcal{H}_{A(B)}$ is not proportional to $H_{A(B)}$. It then follows that the density matrix of GGE, $\rho_{\rm GGE} = Z^{-1}_{\rm GGE}\, {\rm e}^{-(\mathcal{H}_A+\mathcal{H}_B)}$ no longer reduces to a thermal ensemble. Thus, we conclude that the existence of bi-partite entanglement in the initial state is not a sufficient condition for the emergence of asymptotic thermal correlations. An additional condition, such as the existence of a gap, appears to be required.

From the point of view of the theory of critical phenomena, we can regard the existence of a gap as stemming from the presence of a relevant perturbation in the Hamiltonian that is turned off at $t = 0$. This perturbation introduces a characteristic correlation length $\sim \frac{v}{\Delta}$ in the initial state [31] and we may be tempted to associate this fact with the emergence of thermal correlations after the quench. On the other hand, in the above counter-example, what is quenched is a marginal perturbation [31] and therefore, we may conclude, it does not yield thermal correlations. However, this explanation will probably require further investigation and clarification, as we explain in what follows. In the above example, we can consider an initial state that is at finite temperature described by the density matrix $\rho_0 = {\rm e}^{-H_0^{\rm LM}/T}/Z_0$, where $Z_0 = {\rm Tr}\, {\rm e}^{-H_0^{\rm LM}/T}$ and T is the temperature of a thermal reservoir with which the system is in thermal equilibrium at $t \leqslant 0$ (contact with this reservoir is removed at $t = 0$, when $H_0^{\rm LM}$ is quenched to $H^{\rm LM}$). Employing the same methods as in [10], we can evaluate the equal-time single-particle density matrix for the right-moving fermions after the quench, $C_{\psi_R}(x, t > 0) = \langle \psi_R^\dagger(x,t)\psi_R(0,t)\rangle = {\rm Tr}\, \rho_0\, {\rm e}^{{\rm i}H^{\rm LM}t}\psi_R^\dagger(x)\psi_R(0){\rm e}^{-{\rm i}H^{\rm LM}t}$, which reads:

$$C_{\psi_R}(x,t) = \frac{{\rm i}\pi T}{2v_{\rm F}\sinh\left(\frac{\pi T x}{v_{\rm F}}\right)}\left|\frac{\pi T a_0/v_0}{\sinh\left(\frac{\pi T x}{v_{\rm F}}\right)}\right|^{\alpha}, \tag{44}$$

where $\alpha = 2\sinh^2\phi_k$ and a_0 is a short-distance cutoff. Note that, from the point of view of the theory of critical phenomena, finite temperature is a relevant perturbation, which, in equilibrium, changes the asymptotic behavior of correlations in the LM from a power law to an exponential decay characterized by the thermal correlation length $\sim T/v_{\rm F}$ [31]. In the case of a quench, the temperature has a similar effect as in equilibrium. However, in turn, this effect cannot be regarded as leading to effective temperature $\propto T$ due to the presence of the anomalous exponent α in equation (44). This seems to indicate that a large gap introduces a certain type of intrinsically quantum correlations (i.e. entanglement) between the eigenmodes, which are different in nature from the classical correlations due to e.g. temperature, and which, after a quench, manifest themselves as an effective temperature $\propto \Delta$ (see section 2).

4. Discussion and conclusion

In this section, we would like to discuss a number of points concerning the above results. The first point concerns the opposite situation to the one discussed in section 2. We could ask what happens if initially the two subsystems A and B are not coupled and, at $t = 0$, they suddenly become coupled so that entanglement is created. Can we still expect the asymptotic correlations following such a quench to be described by an essentially thermal ensemble in a certain parameter regime? The answer is no, as we explain below.

To address the above question, let us imagine that, initially, the bosons are free to hop everywhere and there is no superlattice. However, at $t = 0$ a superlattice is imposed, say by the sudden application of an extra pair of counter-propagating laser beams. Mathematically, the system at $t \leqslant 0$ is described by the Hamiltonian H (cf equation (20)) and its subsequent evolution at $t > 0$ is described by H_0 (cf equation (19)). The density matrix of GGE is determined by the occupation numbers $n^{\gamma}(k) = \mathrm{Tr}\, \rho_0 \gamma_k^{\dagger} \gamma_k = \sin^2 \theta_k$ and $n^{\delta}(k) = \mathrm{Tr}\, \rho_0 \delta_k^{\dagger} \delta_k = \cos^2 \theta_k$, for a half-filled lattice. Proceeding as above, the GGE density matrix describing the asymptotic correlations is:

$$\rho_{\mathrm{GGE}} \simeq Z_{\mathrm{GGE}}^{-1} \exp\left[\sum_k \frac{\omega_k}{\Delta}(\gamma_k^{\dagger}\gamma_k - \delta_k^{\dagger}\delta_k)\right], \tag{45}$$

for $\Delta \gg 1$. Although the above result may appear to be a thermal ensemble, we must recall the dispersion of the eigenmodes is not $\omega_k = -2\cos k$, but $E_k = \sqrt{\omega_k^2 + \Delta^2}$. Thus, the temperature again becomes mode dependent and equal to $T(k) = E_k \Delta / \omega_k$, which is consistent with the numerical results of [6], where lack of thermalization to the standard Gibbs ensemble but thermalization to the GGE was numerically found in this case.

Thus, it appears again that the emergence of thermal behavior in exactly solvable models requires, at least in the simplest case, the existence of an energy gap in the spectrum of the Hamiltonian that determines the initial state. However, as we have already briefly mentioned in section 2, the thermal ensemble is just an approximation to the more general GGE, which applies in all circumstances. Indeed, the GGE can reproduce the behavior of the asymptotic correlation functions, but it cannot reproduce the behavior of all observables [10]. This is because, in its simplest version of equation (5), the GGE does not capture all the correlations between the eigenmodes that exist in the initial state. For example, in the example of section 2, $\langle I_k I_{k+\pi}\rangle_{\mathrm{GGE}} = \langle I_k\rangle_{\mathrm{GGE}} \times \langle I_{k+\pi}\rangle_{\mathrm{GGE}} \neq \langle \Phi_0 | I_k I_{k+\pi} | \Phi_0\rangle$, where $|\Phi_0\rangle$ is the initial state (i.e. the ground state of H_0, equation (19)) and $I_{k+K} = f_{k+K}^{\dagger} f_{k+K}$. This has important consequences, for example, when considering the energy fluctuations:

$$\sigma^2 = \langle \Phi_0 | H^2 | \Phi_0\rangle - \langle \Phi_0 | H | \Phi_0\rangle^2 \tag{46}$$

$$= \Delta^2 \sum_k \frac{\omega_k^2}{E_k^2}. \tag{47}$$

On the other hand, if we compute the same quantity using the GGE, we find:

$$\sigma_{\mathrm{GGE}}^2 = \Delta^2 \sum_k \frac{\omega_k^2}{2E_k^2} = \frac{1}{2}\sigma^2. \tag{48}$$

As we have shown in section 2, for $\Delta \gg 1$, the GGE tends to a thermal Gibbs ensemble TGE with $T_{\mathrm{eff}} = \Delta/2 = \beta_{\mathrm{eff}}^{-1}$ ($\rho_{\mathrm{GGE}} \to \rho_{\mathrm{TGE}}$). And according to the fluctuation–dissipation theorem, for a thermal ensemble ρ_{TGE} at a temperature T_{eff},

$$C_V = \beta_{\mathrm{eff}}^2 \left.\frac{\partial^2 \ln Z_{\mathrm{TGE}}}{\partial \beta_{\mathrm{eff}}^2}\right|_{V,\ldots} = \frac{\sigma_{\mathrm{TGE}}^2}{T_{\mathrm{eff}}^2}, \tag{49}$$

where C_V is the heat capacity of the system. Yet, the actual energy fluctuations of the system following a quantum quench in which a superlattice of strength $\Delta \gg 1$ is turned off at $t = 0$ are given by $\sigma^2 = 2\sigma_{\mathrm{GGE}} \simeq 2\sigma_{\mathrm{TGE}}$ (cf equation (48)). Therefore, we conclude that the fluctuation–dissipation theorem breaks down in the model of section 2, in spite of the fact that the asymptotic correlations appear to be essentially thermal for $\Delta \gg 1$. Therefore, the effective temperature does not have the same meaning in the thermodynamic sense; it is the temperature that determined the correlations in the system and it is also a measure of the entanglement between the eigenmodes in the initial state.

Nevertheless, although the effective temperature obtained in equation (33) has no thermodynamic meaning in the sense of the fluctuation–dissipation theorem, it still represents a quantity that is worth determining experimentally. The reason is that $T_{\rm eff}$ is a measure of the entanglement in the system. Indeed, determination of $T_{\rm eff}$ from, say, a measurement of the boson momentum distribution, should allow for a determination of the entanglement spectrum of $\mathcal{H}_{A(B)}$, which, according to the discussion in sections 1 and 2, is given by $\mathcal{H}_{A(B)} \simeq H_{A(B)}/T_{\rm eff}$. Thus, an experimental determination of the von Neumann entropy, $S_{A(B)} = -{\rm Tr}\, \rho_{A(B)} \log_2 \rho_{A(B)}$, ($\rho_{A(B)} = {\rm e}^{-\mathcal{H}_{AB}}/Z_{A(B)}$) would also be possible. For $\Delta \to \infty$, the effective temperature also goes to infinity, then $S_A = N$ if there are N different k modes. In this case, the infinite coupling between two chains produce N maximum entangled states between each k mode, and the entanglement entropy S_A measures how many maximum entangled states there are between the two subsystems. The same principle applies to finite Δ and thus finite temperature. Similar remarks are applicable to the counter-example discussed in section 3, provided we exchange the role of $T_{\rm eff}$ by ϵ. In this case, however, we cannot expect thermal correlations.

In summary, we have presented a simple instance of a quantum quench in which a quantum quench in an exactly solvable system can produce essentially thermal correlations. The emergence of thermal correlations from the GGE has been related to the existence of bi-partite eigenmode entanglement and a gap in the spectrum of the Hamiltonian that describes the initial state. In this regard, we have also discussed a counter-example demonstrating that thermalization does not happen if the initial state is described by a gapless Hamiltonian. Our results allow us to establish a link between the GGE and the entanglement spectrum in exactly solvable systems with bi-partite entanglement of the eigenmodes. Thus, it makes possible an experimental measurement of the entanglement spectrum and other quantities derived from it (such as the von Neumann entropy), provided the asymptotic correlation functions of the system following a quantum quench can be measured experimentally. We have argued that this task becomes particularly simple when the GGE reduces to a thermal ensemble (or, when the entanglement spectrum has a relatively simple form, as in the counter-example discussed in section 3). Whether this connection between entanglement and thermal correlations is generic, that is, it applies to systems other than the exactly solvable models that can be treated by the methods of [12], is a matter for future research. Finally, we have also shown that, even if correlations may become essentially thermal, other quantities, such as the energy fluctuations, are not. This is akin to a breakdown of the fluctuation–dissipation theorem.

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Appendix. Quantum quenches in the sine-Gordon model

The sine-Gordon model has been introduced in the main text (see equation (34)). This model has an exactly solvable point at $K = 1$ (the so-called Luther–Emery point), at which the Hamiltonian of equation (34) can be conveniently represented as a quadratic form of fermion fields. To this end, we must use the following bosonization identity:

$$\psi_\alpha(x) \sim \frac{1}{\sqrt{2\pi a}}\, \mathrm{e}^{\mathrm{i}s_\alpha \phi_\alpha(x)}, \tag{A.1}$$

where we have introduced the index $s_\alpha = 1$ for $\alpha = R$ and $s_\alpha = -1$ for $\alpha = L$, and the chiral bosonic fields $\phi_\alpha = K^{-1/2}\phi + s_\alpha K^{1/2}\theta$, and $\psi_{R,L}$ are destruction operators for spinless fermions moving to the right and to the left, respectively. Using the above identity and, after a Fourier transformation, the Hamiltonian becomes:

$$H_{\mathrm{sG}} = \sum_p \varepsilon_p^0 \left[\psi_{\mathrm{R}}^\dagger(p)\psi_{\mathrm{R}}(p) - \psi_{\mathrm{L}}^\dagger(p)\psi_{\mathrm{L}}(p)\right] + \Delta \sum_p \left[\psi_{\mathrm{R}}^\dagger(p)\psi_{\mathrm{L}}(p) + \psi_{\mathrm{L}}^\dagger(p)\psi_{\mathrm{R}}(p)\right], \tag{A.2}$$

with linear dispersion $\varepsilon_p^0 = vp$.

Let us consider a quench in which the system is initially prepared in the gapped ground state of H_{sG}, or more generally, in a thermal state defined by a density operator $\rho = \mathrm{e}^{-H_{\mathrm{sG}}/T}$ with temperature T. We then assume that the coupling g is suddenly turned off at $t = 0$, and therefore, for $t > 0$ the time evolution is governed by H_0. In the long times regime, the expectation value and correlations of a broad class of operators for long times can be described by the GGE [32].

The sine-Gordon Hamiltonian at the Luther–Emery point can be diagonalized by the Bogoliubov transformation

$$\psi_{\mathrm{R}}(p) = \cos\theta_p \psi_c(p) - \sin\theta_p \psi_v(p), \tag{A.3}$$

$$\psi_{\mathrm{L}}(p) = \sin\theta_p \psi_c(p) + \cos\theta_p \psi_v(p) \tag{A.4}$$

provided we choose

$$\tan 2\theta_p = \frac{\Delta}{\varepsilon_p^0}. \tag{A.5}$$

In terms of the new variables $\psi_{v,c}$ it turns out to take the diagonal form

$$H_{\mathrm{sG}} = \sum_p \varepsilon_p \left[\psi_c^\dagger(p)\psi_c(p) - \psi_v^\dagger(p)\psi_v(p)\right]. \tag{A.6}$$

with dispersion $\varepsilon_p = \sqrt{[\varepsilon_p^0]^2 + \Delta^2}$. This Hamiltonian is a continuum version of the superlattice model discussed in section 2, which is obtained from (19) in the limit where $k = p \to 0$.

For an initial thermal state, the eigenmode occupations are:

$$\langle \psi_{\mathrm{R}}^\dagger(p)\psi_{\mathrm{R}}(p)\rangle = \frac{1}{2}\left(1 - \cos 2\theta_p \tanh\frac{\varepsilon_p}{2T}\right), \tag{A.7}$$

$$\langle \psi_{\mathrm{L}}^\dagger(p)\psi_{\mathrm{L}}(p)\rangle = \frac{1}{2}\left(1 + \cos 2\theta_p \tanh\frac{\varepsilon_p}{2T}\right), \tag{A.8}$$

and hence the values of α and β that determine the GGE read:

$$\alpha(p) = \log\left[\frac{1-\cos 2\theta_p \tanh\frac{\Delta}{2T}}{1+\cos 2\theta_p \tanh\frac{\Delta}{2T}}\right], \tag{A.9}$$

$$\beta(p) = \log\left[\frac{1+\cos 2\theta_p \tanh\frac{\Delta}{2T}}{1-\cos 2\theta_p \tanh\frac{\Delta}{2T}}\right]. \tag{A.10}$$

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